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Youngstown State University
410 Wick Avenue
Youngstown, OH. 445550001

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TITLE OF PROPOSED PROJECT

RUI - Cooperative Research Project - Structural Investigations of Main Group Heterocyclic Rings and Cages

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PREPROPOSAL NO., IF APPLICABLE
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Received :04/28/2000

CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

(1) the statements herein (excluding scientific hypotheses and scientific opinions) are true and complete, and
(2) the text and graphics herein as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or individuals working under their supervision. I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this proposal.

I understand that the willful provision of false information or concealing a material fact in this proposal or any other communication submitted to NSF is a criminal offense (U.S.Code, Title 18, Section 1001).

Name (Typed)	Signature	Social Security No.*	Date
PI/PD **Allen D Hunter**			
Co-PI/PD			
Co-PI/PD			
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Co-PI/PD			

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Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding Federal debt status, debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in Grant Proposal Guide (GPG), NSF 00-2. Willful provision of false information in this application and its supporting documents or in reports required under an ensuring award is a criminal offense (U. S. Code, Title 18, Section 1001).

In addition, if the applicant institution employs more than fifty persons, the authorized official of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of Grant Policy Manual Section 510; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflict which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF.

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This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding $100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding $150,000.

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The undersigned certifies, to the best of his or her knowledge and belief, that:

(1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

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This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME/TITLE (TYPED) **Dr. Peter J. Kasvinsky/Graduate Dean**		**04/28/00**

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Received :04/28/2000

Section A: Project Summary

This proposal describes a collaborative research project that has two synergic components, one focuses on the scholarship of diffraction education and the other on the utilization of advanced diffraction methods in chemical research. Dr. Allen D. Hunter of Youngstown State University will spend his first sabbatical working with Drs. J. Derek Woollins and Alex Slawin of St. Andrews University. Dr. Hunter's expertise in diffraction methods education will be emphasized during the first 4 month phase of this project when he will prepare a variety of teaching materials aimed primarily at undergraduates. These will then be pilot tested and revised at St. Andrews University where a WEB site mirror of his online teaching materials will also be placed. During the second 7-8 month phase of his sabbatical, Dr. Hunter will be involved in the integration of high resolution diffraction methods into the study of Dr. Woollins' main group inorganic and organometallic ring and cage complexes. This data will be collected on Drs. Woollins' and Slawin's two new CCD diffractometers and on the CLRC synchrotron at Daresbury. In collaboration with Dr. Slawin, a combination of charge density, molecular orbital, and molecular mechanics calculations will be used to rationalize the structures and bonding of these materials in the solid state and their spectroscopic properties in solution. Funding for the education research phase of this project is being primarily provided by Youngstown State University and St. Andrews University and by the participants' current NSF-DUE-CCLI-EMD and UK – EPSRC grants. The NSF International Division funding being requested is to support the incremental costs of the second phase of this project, namely: the development of the long term collaborative research project. The results of this sabbatical will reinvigorate the PI's research program when he returns to YSU, a predominantly undergraduate institution, where this type of diffraction study makes ideal undergraduate student research projects. The knowledge and experience gained in the areas of main group chemistry and charge density, molecular orbital, and molecular mechanics methods will also be integrated into the undergraduate and graduate curricula at YSU and into his diffraction teaching materials.

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For font size and page formatting specifications, see GPG section II.C.

*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

Section C: Project Description

C1 Results From Prior NSF Support[1-11]

C1a NSF DMR 9403889: "Acquisition of a Single Crystal X-Ray Diffractometer"

This *research equipment* grant ($71,199, ≈ $200,000 match, 1994-96, T. Wagner PI and **A. Hunter**, J. Jackson, and R. Beiersdorfer Co-PIs) was funded for one P4 diffractometer but with extra matching funds it was used to purchase 2 new Siemens (now Bruker-AXS) P4 X-ray diffractometers, a LT2 low temperature attachment, a X-1000 multi-wire area detector, and a number of SGI and PC workstations for data processing (these have been supplemented/upgraded several times). These acquisitions have allowed integration of advanced diffraction methods into the junior/senior level chemistry curriculum at YSU.[4-7] A new 3 quarter hour course, "Chemistry 832: Solid State Structural Methods," that fully integrates this equipment is offered each year and its students include many non-chemistry majors (e.g., from engineering and geology). It is being converted to a 3 semester hour course, Chemistry 5832, for Spring of 2001. It has directly led to papers with undergraduate co-authors,[10] a laboratory manual,[5] and presentations at national crystallographic education[6] and regional science education[7] meetings. Powder and single crystal diffraction methods have also been integrated into five other upper level chemistry courses[4-7] and this instrument has been used by faculty and students from several regional liberal arts colleges.

C1b NSF DUE 9850079: "Investigative Approaches in the Natural Sciences"

This *DUE* grant ($183,579, ≈ $200,400 match, 1998-2001, J. Usis PI and **A. Hunter** and C. Singler Co-PIs) is being used by a multidisciplinary team to develop a new lab course, Arts & Sciences 2600, having collaborative "research like" projects. It is designed to teach students what science is by having them do science. Starting this August, it will be required of all non-science and non-technology majors at YSU (i.e., to satisfy the natural science lab requirement in the new general education program). This course has been pilot tested several times and over a dozen sections will be offered each semester starting this coming Fall. It has also being discussed as a model course for other Ohio Universities.[7]

C1c NSF DUE ILI 9851107: "Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment"

These *ILI* grant funds ($44,600, over $44,600 match, 1998-2001, **A. Hunter** PI and S. Brower, T. Kim, D. Mincey, and T. Wagner Co-PIs) have been stretched to purchase more capable instrumentation then originally proposed, including: (a) a TA Instruments 2910 DSC, a 2050 TGA, a data system, and an upgrade of our older Dupont DSC/DMA/TMA data system, (b) a Cannon CT-518 constant temperature bath, and (c) a GBC Instruments/Polymer Labs GPC-SEC-HPLC system (i.e., autosampler, isocratic/gradient pump, column oven, RI and diode array UV-visible detectors, and data system) as well as additional equipment (authorized by Susan Hixson, DUE, January 1999) including: (d) a Jasco 410 FT-IR (0.9 cm^{-1}) and (e) a Vacuum Atmospheres HE-43-2 inert atmosphere glove box with the residual funds. These instruments have now been integrated into 6 upper division Chemistry and Chemical Engineering courses and into undergraduate research and over the coming months its integration into several lower division Chemistry courses and into the Condensed Matter Physics course will be completed. These efforts are facilitating interdepartmental collaborations as well as the integration of materials science into non-specialist courses.

C1d NSF DUE 9551683: "Integration of GC-MS into the Undergraduate Curriculum"

This *ILI* grant ($34,450, ≈ $50,000 match, 1995-96, J. Jackson PI and **A. Hunter**, S. Schildcrout, R. Falconer, and T. Wagner Co-PIs) was used to purchase a Finnigan 1020 Gas Chromatograph-Mass Spectrometer which has subsequently (Dec. 1999) been upgraded with a new system controller, data system, and software. This instrument is now fully integrated into student research, senior level Organic Synthesis, Organic Analysis, Physical, and Inorganic Lab courses (i.e., 50 students a year), and into the Sophomore Organic sequence (i.e., ≈ 200 students a quarter, primarily from the natural sciences, engineering, and pre-medicine). In each case, it has facilitated a new collaborative learning/discovery-oriented approach.[8,11] Our success with integrating this and related instruments into our teaching and student research sufficiently impressed an Ohio Board of Reagents review panel that they recently helped fund a new LC-MS on campus.

C1e NSF DUE-CCLI-EMD-POC "X-Ray Diffraction Analysis Throughout the Curriculum: a Powerful Tool for Understanding Molecular Structure and Bonding"

This *DUE Educational Materials Development Grant* ($74,707, 2000-02, **A. Hunter** PI) was recently awarded and the starting date is May 1st, 2000. It proposed the development of new documentation (texts and/or Adobe PDF), software, and other teaching materials to enhance the integration of single crystal diffraction methods into the undergraduate curriculum. More discussion of this project is given below as it directly relates to the first phase of the current proposal. A copy of this proposal is available at: http://www.as.ysu.edu/~adhunter/YSUSC/EMD1999Prop.pdf

C1f Other Science Education Grant Support

The PI and his Youngstown State University colleagues have been very active in the field of science education. In addition to the above NSF grants involving the PI, several other grants have recently (over the last 4 years) been awarded to the PI and his colleagues from non-NSF sources and to his YSU Chemistry colleagues from NSF sources to support science education. These efforts have included NSF funds to revitalize our General Chemistry sequence (NSF-DUE-CCLI-A&I #9981040, T. Wagner PI and J. Mike Co-PI) and our Analytical/Environmental sequences (e.g., NSF-DUE-ILI #9751151, D. Mincey PI and R. Falconer, T. Wagner, and S. Martin Co-PIs). We have also received four highly competitive Ohio Board of Regents grants for Chemistry Computer Labs and Instrumentation for Undergraduate Research and Education including diffraction, NMR , and LC-MS instrumentation (**A. Hunter** Co-PI on the computer grant and **A. Hunter** YSU PI on the Instrumentation grants). All of these educational initiatives involve close collaborations across campus, especially with the Environmental Studies and General Education programs and with the departments of Biology, Geology, Math, Physics, and Civil and Chemical Engineering.

Our Department's interested in the scholarship of science education has recently lead to our decision to build a formal Chemistry Education division. We recently hired Stacy Lowery-Bretz from the University of Michigan who is an expert on science education and assessment and are hoping to soon hire a second science education faculty member to be jointly appointed with our College of Education. These individuals are expected to have a substantial impact on educational initiatives, especially on the assessment of curriculum changes and student learning outcomes.

C2 The Rationale for and Benefits to be Derived from International Collaboration

C2a Youngstown State University and its Chemistry Department

Youngstown State University is an *open enrollment* public university located in downtown Youngstown. Youngstown is located about half way between Pittsburgh and Cleveland in Northeast Ohio and is a former steal making center whose economy has only recently begun to recover. We currently enroll approximately 12,000 undergraduates. These students pursue a combination of 1 and 2 year Associate Degrees and 4 year Bachelors Degrees from our Colleges of Art & Sciences, Business, Education, Engineering, Health & Human Services, and Fine & Performing Arts. Our students are typically in the first generation in their families to attend college, they work an average of 30 hours a week to support their educations, and greater than 90% commute to campus. Indeed, we have an above average proportion of "non-traditional" college students.

Although YSU also has masters level programs in about two dozen disciplines, including Chemistry, Biology, and Math (which award research based MS degrees), it does not award PhD degrees in any NSF supported field. Youngstown State University is therefore officially designated as a **Predominantly Undergraduate Institution**.

Our Chemistry Department has 15 full time faculty, all with PhDs in Biochemistry, Chemistry, or Chemical Education. We also have several PhD level Adjunct Faculty and Affiliated Scholars who are employed at regional community and liberal arts colleges, in government labs, or in industry. They have full access to our facilities and participate in our departmental teaching and student research missions. We have three full time support staff, including an office manager, a purchasing and chemical safety officer, and an electronic instrumentation specialist. We also make extensive use of students in these support functions.

Our department has established divisions of Biochemistry and Analytical, Inorganic, Organic, and Physical Chemistry and is just in the process of adding a Division of Chemical Education. We offer BA, BS (ACS approved), and MS degrees in Chemistry. Our Departmental Goal is to be one of the *Top Ten MS level Institutions in the US*. In his recent external program evaluation, Dr. Conrad Stanitski (an ACS evaluator from Central Arkansas University, 1998) indicated that we were on the threshold of reaching this goal. Indeed, we are now arguably one of the best equipped non-PhD department in the US. We graduate approximately 30-40 undergraduates (BA and BS) and 5-10 MS students each year. The large majority of our BS and MS graduates proceed on to *top ranked* PhD programs or are *snapped up* by industry. We have built a very strong reputation for producing students that have both good class room knowledge but also truly outstanding "hands on" experience. Thus, our BS students typically have extensive "hands on" experience operating a wide range of analytical and spectroscopic instrumentation, including research grade MS, NMR, IR, and Diffraction system. We also collaborate closely with other YSU science and engineering departments and with the College of Education (with whom we are strongly involved in revitalizing science education at the pre-college level in our region).

C2b The PI's Balance Between Science Education vs. Chemical Research

As can be seen from the above discussion, from his Biographical Sketch (section E, pages E1/E2), and from his Current and Pending Support form (section G, pages G1/G2), the PI has become increasingly involved in Science Education and the funding of Research/Educational Instrumentation (i.e., he is the Director of the YSU Structure Center) over the last 6 years. This has lead to an increasing stream of oral presentations,[6,7] publications,[4,5,8,9] and educationally related grants. Indeed, he is currently scheduled to give 10 papers on these topics at national and international meetings over the next year, he has been invited to write a text book, and his

educational/instrumentation grant total is now approaching $900,000 since 1994 (i.e., as PI or major Co-PI). In turn, these activities has lead to some regional, national, and even international prominence in these areas (see, for example, page E2 – Synergistic Activities). This success strongly contributed to his recent promotion to Full Professor at YSU and has enriched the teaching and learning environment for YSU students.

This professional growth in the area of educational scholarship has come, to a substantial extent, at the expense of his activity in the area of conventional chemical research. Over these same 6 years, his conventional research productivity has dropped from approximately 3-4 peer reviewed publications a year to something closer to one.

Since there is substantial synergy between active scholarship in ones discipline and the scholarship of teaching, this current imbalance between conventional research and teaching will eventually adversely impact his teaching. In addition, the PI does not want to be so heavily focused on one aspect of his scholarly activity. He would like to move from the current 4:1 ratio in favor of the scholarship of teaching towards a more equal balance of 2:3 favoring chemical research. Finally, it is challenging to remain current in ones discipline in a predominantly undergraduate institution and sabbaticals are an excellent way of reentering the mainstream of research. It was in recognition of these needs, that the PI applied to Youngstown State University last fall for a sabbatical for 2000/2001. This application emphasized the synergy of teaching and research in crystallography but had its predominant thrust in the area of diffraction research. YSU has acknowledged the desirability of this refocusing of his efforts and expertise by granting him a sabbatical at St. Andrews University for this project.

C2c Why Overseas and Why St. Andrews?

The US has many excellent crystallographers. Indeed, the PI has collaborations with several of them listed on his Biographical Sketch. Therefore, the obvious question is why the PI decided to take his sabbatical overseas. The answer to this question has several parts. Firstly, no appropriate sites in the US are within daily commuting distance of the PI's home (the closest are approximately 200 miles away at the University of Toledo and at SUNY Buffalo). To become fully immersed in this project, the PI would therefore have to move his family for the duration. Once that decision was made, it became clear that the actual incremental cost of such a move, and hence maintaining a second residence, was almost independent of the region of the target move (the variations being primarily dependent on housing costs and the level of local sabbatical support). This lead to the conclusion that the PI should chose a sabbatical location that was maximally beneficial to his sabbatical educational and research goals.

The educational goals of the sabbatical project required a host with a substantial commitment to revitalizing the way undergraduates are taught diffraction methods. To meet the research goals, this host also needed to have an interest in studying inorganic materials by charge density methods. Finally, the host institution needed to have a community of crystallographic experts on site and had to have sufficient free diffractometer time available to enable the PI to carry out his planned studies. This combination of requirements narrowed the pool of possible sabbatical sites down considerably. Potential hosts at several dozen such sites at which the PI had contacts in the US and internationally were then contacted about his sabbatical plans. Several of these expressed a greater or lesser degrees of interest in hosting the PI's sabbatical.

Professor Woollins of St. Andrews University expressed the greatest degree of interest in hosting the PI for his sabbatical. He and the PI have similar interests in crystallographic education. Indeed, Dr. Woollins was one of the earliest adopters of the PI's diffraction methods lab manual[5] and Dr. Woollins invited the PI to write a Tutorial Text on Diffraction Methods for Novices (i.e., for a Royal Society series he is editing). Drs. Woollins and Slawin were also interested in applying modern charge density methods to Professor Woollins' main group

compounds to help explain some unexpected structural, reactivity, and spectroscopic properties. This level of interest was so great that Dr. Woollins was willing to allocate £6,000 from his existing UK – EPSRC (Engineering and Physical Sciences Research Council) grants to partially support the PI on his sabbatical. None of the other sites expressed a similar enthusiasm for the PI's project which blends teaching and research objectives.

There are several reasons why an international site was, in any case, preferable for the educational component of this project. The most compelling of these is that the PI would like to integrate the best of the US and foreign approaches to undergraduate education, which can be quite different, into his new teaching materials. These educational differences arise from the US emphasis on liberal education vs. the European tradition of more professionally focussed university studies. [Note: The YSU sabbatical review committee felt that the choice of a foreign sabbatical site was one of the stronger parts of the PI's sabbatical application.] The PI had previously taught in Canada (i.e., as a Teaching Assistant at University of British Columbia and as an Assistant Professor at the University of Alberta) and had observed the Australian system during his post-doctoral stay there (i.e., at the Australian National University). He was particularly interested in observing/participating in the European approach to undergraduate education (especially as it relates to diffraction methods) and having a European base would substantially facilitate this goal. To this end, St. Andrews' Scottish location is ideal. In fact, the PI is already committed to participating at various crystallographic education forums during the coming year, including examples in: Scotland and England (which have surprisingly different educational systems), France, Germany, and Spain.

Considering this combination of factors, the PI felt that St. Andrews University, which has a particularly strong group of crystallographers and crystallographic facilities, was *the best all around location for his sabbatical*.

C2d Benefits of this New Trans-Atlantic Collaboration

At the completion of this project, the PI and his undergraduate research students will benefit by his being better prepared to carry out cutting edge crystallographic research involving charge density and molecular mechanics/orbital calculations at Youngstown State University. He will also have established the ground work for a long term research collaboration with Drs. Woollins and Slawin involving the study of main group inorganic and organometallic rings and cages. Main group inorganic chemistry is an area where the PI has had little previous practical experience. This main group metals, charge density, and molecular mechanics/orbital experience will be integrated into his teaching back at YSU.

The students at St. Andrews University will benefit by becoming more involved in the crystallographic education research. It will be a primary test site for the PI's new crystallographic education materials and will be the lead institution in the European dissemination of these materials. Finally, the research groups at St. Andrews will benefit from the PI's participation in their research projects.

C3 Research Objectives

C3a Crystallographic Education and Research: A Natural Synergy

Many recent national studies and publications have noted the natural synergy between teaching and research.[12] As noted above, this collaborative project is designed to exploit these synergies when applied to diffraction methods. The new knowledge and practical research experience that the PI gains will beneficially impact both his crystallographic education and undergraduate student research projects. In turn, the PI will assist with updating some aspects of the St. Andrews University curriculum as well as contributing to the attainment of the research goals of the Woollins and Slawin groups.

While the PI expects to work on both facets of this project throughout his stay at St. Andrews University. The first 4 months will emphasize the crystallographic education project (driven largely by the approaching deadline for his text in this area and the need to complete the first draft of the teaching materials for α-testing (i.e., for use in the Spring of 2001)). The last 7-8 months will emphasize crystallographic research. The PI will spend part of the first phase learning crystallographic techniques new to him for inclusion in his teaching materials. This new familiarity will also speed his charge density research once his focus shifts to this topic in December.

C3b Crystallographic Education Projects from the PI's Group

Recent changes in computer and crystallographic hardware technology and in diffraction theory and software have led to a *simultaneous* increase in both *ease of use* and *power* of single crystal diffraction methods. Because of these changes, the number of single crystal diffraction analyses being carried out has increased incredibly rapidly. This has lead to a change in who carries out such studies. No longer are they done almost solely by crystallographic professionals. Rather, an increasing number of non-experts are getting involved in the collection of crystallographic data and the solution of single crystal structures, especially for more routine examples.[6c,13,14] Indeed, a diverse array of individuals including synthetic chemists, biochemists, structural biologists, geologists, materials scientists, etc., now use diffraction methods as a regular part of their research.[4,6,7] While many crystallographers have observed this trend with trepidation, it continues to gain steam. In fact, this trend towards non-experts using crystallography as another tool is actually no different than how such individuals have long used spectroscopic methods such as NMR (whose theoretical basis is arguably as, or more, difficult to master). This has lead to a rapid increase in the need for *appropriate* crystallographic training for these individuals and hence the development of teaching tools aimed at a much broader audience than was common in the past.[4-7,13-15]

The PI has been a significant participant in developing such crystallographic education materials. His area of special emphasis is the development of crystallographic education materials aimed at novice users such as undergraduates.[4-7] He recently wrote a proof of concept proposal to the NSF-DUE-CCLI-EMD program to fund his work in this area. This proposal was entitled "X-Ray Diffraction Analysis Throughout the Curriculum: a Powerful Tool for Understanding Molecular Structure and Bonding" (NSF #9980921) and was recently funded ($74,707, 05/01/2000 – 04/30/2002). The central goal of this project is to develop a series of teaching materials to enable the better integration of diffraction methods into science lab (computer and instrumental) curricula. These materials are to include at least one text (for the Royal Society's "Tutorials in Chemistry" series, J. Derek Woollins, Editor), instructor and student handouts and training materials, tested laboratory modules, a WEB database of annotated structural data, and one or more free "student editions" of commercial diffraction analysis programs (developed in collaboration with diffractometer vendors).

These teaching materials are being developed at several levels of sophistication. The most elementary level will most likely be used in General Chemistry and high school chemistry. It has an emphasis on using hands on solution of structural problems to reorganize how molecular structure and bonding are taught (i.e., toward a collaborative discovery based model). The intermediate materials are designed to be inserted as modules into current courses such as Intermediate Inorganic, Organic Analysis, Structural Biochemistry/Biology, Mineralogy, Materials Science, etc. The most advanced materials are designed to be used in dedicated introductory diffraction methods courses aimed at novices such as undergraduates and non-specialist graduate students. The team that is doing this work includes YSU students and several regional high school chemistry teachers. The early versions of some of these materials have already been found useful and the new materials will be more widely tested by already identified individuals at several dozen other colleges and universities and at regional high schools.

C3c Crystallographic Education Objectives of this Collaborative Project

At St. Andrews, the PI will concentrate on crystallographic education objectives for the first third of his sabbatical. He has several specific objectives in mind for this August to November period, namely:

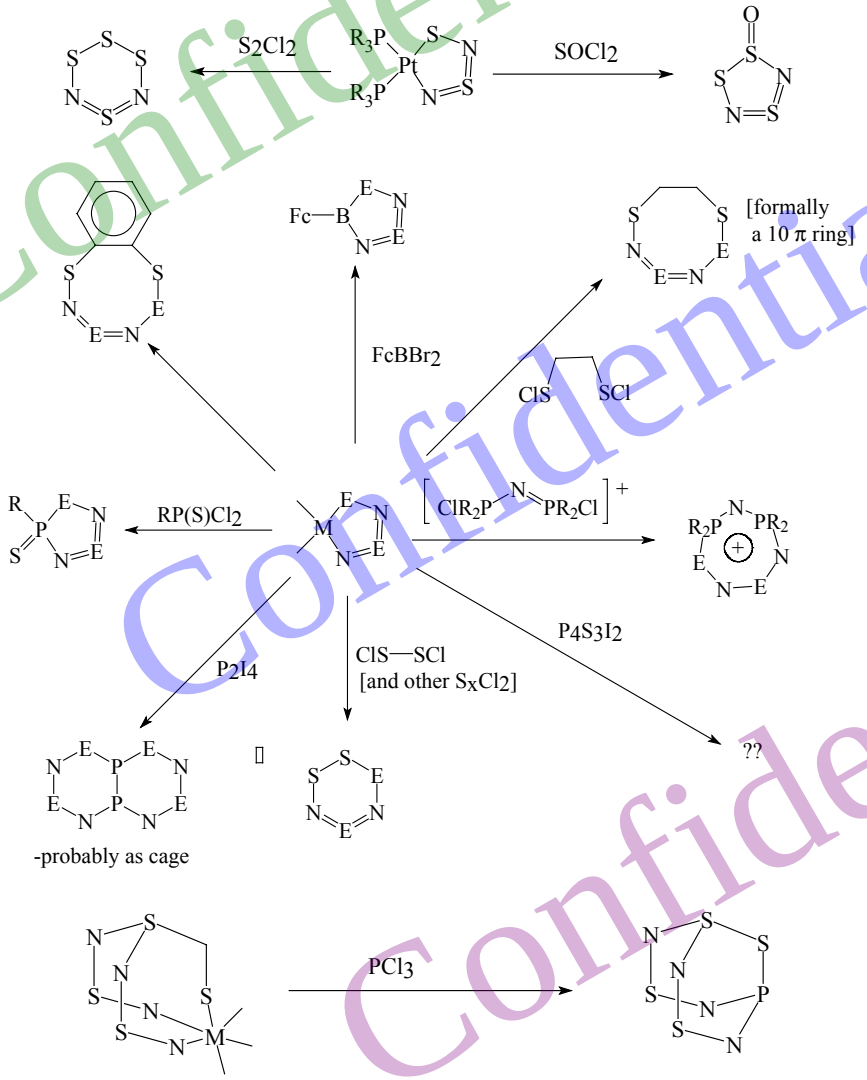
- While the PI is quite familiar with serial diffractometers, he has had little experience with area detector systems such as CCDs. By carrying out some conventional CCD crystal structure determinations, he will become proficient with the new Bruker-AXS and Rigaku-MSC CCD systems in the Woollins/Slawin labs. He will also practice (less extensively) with one of the Imaging Plate systems at St. Andrews.
- He will incorporate information on these increasingly common and important CCD and Imaging Plate detector types into his teaching materials.
- He will complete a draft of his RSC "Tutorials in Chemistry" text: *"Single Crystal X-Diffraction Analysis for Novices"* for evaluation and suggestions from the Royal Society's reviewers.
- He will complete the preliminary drafts of the entry level teaching materials (i.e., developed over the summer of 2000 by his team) and pilot test them with St. Andrews students while his collaborators in Youngstown do the same with US students. He will then revise and distribute them electronically to high schools and colleges and universities for α-testing during the Spring of 2001.
- Based on the features identified over the summer as necessary for the student exercises/projects, he will complete work with the commercial software vendors on the "student editions" of their diffraction analysis software packages (two have currently decided to participate).
- He will complete the first stage of the WEB site (to be mirrored at Youngstown State University and St. Andrews University) containing at least 50 annotated diffraction data sets previously collected at St. Andrews.
- The results of these phase one educational efforts will be disseminated via conference presentations in at least 5 European countries and articles in the British Crystallographic Association and ACA/IUCr/Pittsburgh Diffraction Society newsletters.

Note: Funding to support this diffraction education initiative is not being sought in this current NSF – International Division proposal. They have already been committed from Youngstown State University, J. Derek Woollins and St. Andrews University, and a NSF-DUE-CCLI-EMD grant, see section C6, below.

C3d Main Group Chemistry Research from the Woollins / Slawin Groups

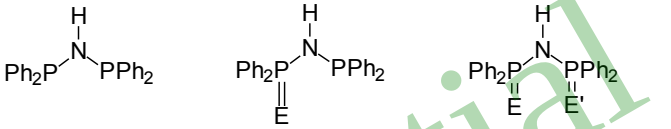
Main group inorganic compounds are both interesting in their own right and for their applications to other areas of chemistry. A central theme of main group chemistry has been to explore the wide structural diversity and reactivity of these materials, especially their abilities to form complex rings and cages.[16] One major use of these materials is as ligands for transition metal complexes and catalysts.[17] A second is their use as reagents in organic synthesis.[18] A third is their use in the synthesis of solid state materials.[19] Dr. Woollins is an international leader, and has an extremely active research program, in each of these areas. Indeed, his research is funded by the UK – EPSRC (Engineering and Physical Sciences Research Council) and industry to the tune of over $250,000 per year.

C3d(i) Synthesis of Main Group Rings and Cages: Group 15 elements such as N and P in combination with group 16 elements such as O, S, Se, and Te form a wide variety of products displaying inorganic ring and cage structures. Recent work funded by the UK – EPSRC in the Woollins group focuses on using transition metal – main group ring compounds to synthesize novel main group inorganic ring and cage species, for example:[20]

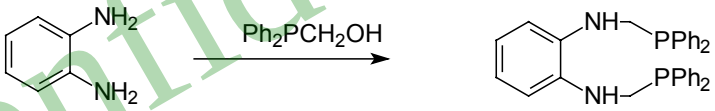


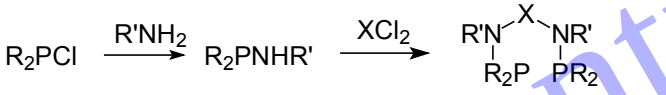
These compounds are interesting in their own right, for use as reagents and/or catalysts, and for use as precursors for inorganic polymers and solids.

C3d(ii) Main Group Ligands and Transition Metal Chemistry: Many of the most important ligands in transition metal inorganic and organometallic chemistry traditionally have contained N or P binding sites or O or S binding sites. The Woollins group is funded by the UK – EPSRC and industry to develop better routes to current ligands and new ligand structures having a combination of such binding sites (especially those with both hard and soft Lewis Base centers), for example:[21]



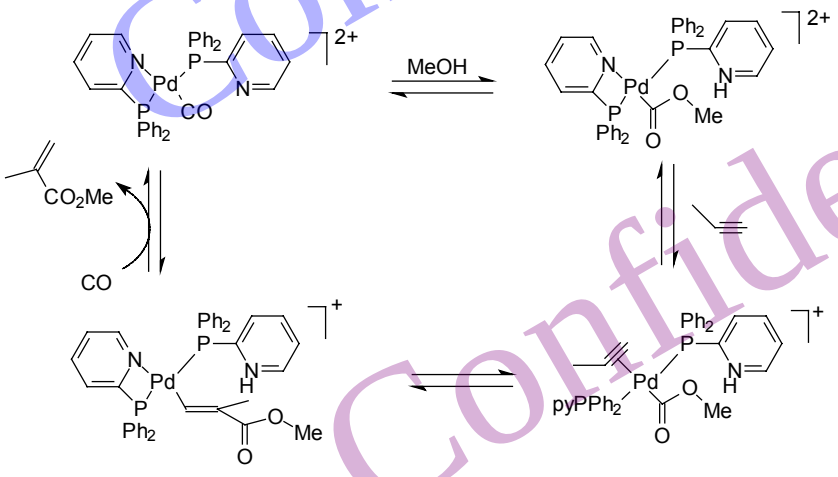
E = O, S, Se; E' = O, S, Se





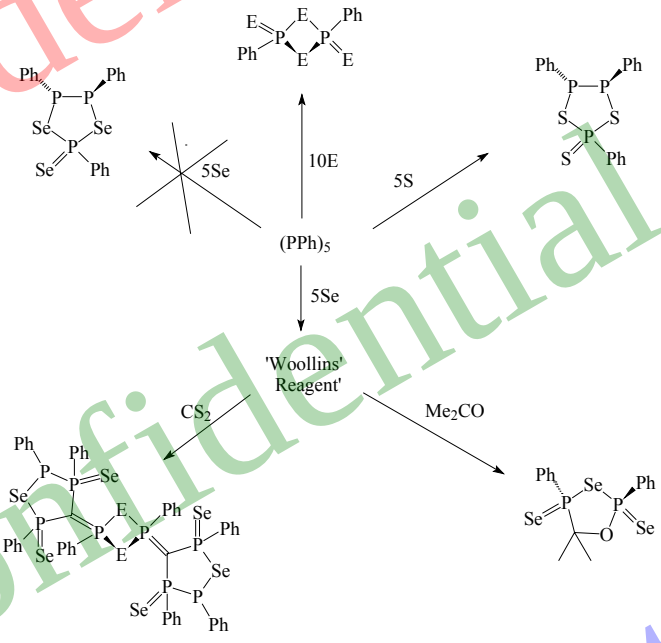
X = S, SO, SO_2, Se, Te, PR, AsR, Me_2Si, RB, Cp_2Ti, Cp_2Zr

They also study the use of such ligands in catalytic reactions, for example:



Finally, they have described some of these reactions for teaching publications.[22]

C3d(iii) Main Group Compounds in Organic Chemistry: Many key organic transformations involve main group reagents. The Woollins groups is funded by the UK – EPSRC to develop and investigate such reagents. One current project focuses on the "Woollins Reagent" (i.e., related to Lawessons Reagent) both in identifying its structure and developing its utility in organic and main group chemistry, for example:[23]



C3d(iv) Main Group Compounds in Materials Chemistry/Science: Many industrially important and scientifically interesting extended and molecular solids contain components that are rich in elements in groups 15, 16, and 17. In work funded by the UK – EPSRC and industry, the Woollins group is interested in finding improved routes to know solid state materials as well as in engineering[19] new solid state materials. For example, they are preparing main group inorganic ring and cage complexes as precursors to extended solids rich in atoms such as S and Se. They are also preparing new molecular solids having novel combinations of organic bases and large inorganic counter ions (e.g., (Bis(ethylenedithio)tetrathiafulvalene)$_5^{\bullet}$($B_{10}I_{10}$)).[24]

C3d(v) Characterization of these Main Group Compounds: Once these new main group inorganic and organometallic materials have been prepared and purified, they must be characterized. One aspect of this is the study of the study of their stoichiometric and catalytic reactivities. The other is the determination of their physical,[25-27] analytical and spectroscopic,[28] and crystallographic[15,29] properties. These types of information are used to characterize the structures and bonding of such materials in the solid state and solutions. This, in turn, can be used to rationalize (and later optimize) their reactivities and their physical properties (e.g., electrical conductivity). While Dr. Woollins' students typically do their own analytical and spectroscopic studies (sometimes in collaboration with the St. Andrews or external service staff or with external researchers), it is Dr. Slawin and her group who characterize their solid state structures. The larger and more strongly diffracting crystals have their diffraction data collected on one of the diffractometers in the Woollins/Slawin lab while the smaller and more weakly diffracting crystals have their diffraction data collected at the CLRC synchrotron facility at Daresbury. A central part of these groups' activities lies in relating these various types of data.

One of the most scientifically interesting classes of questions come where one or more of these methods gives conflicting results. It is in elucidating what is happening in these cases that high resolution diffraction data and the resulting charge density and molecular orbital and mechanics studies offer their promise.[30]

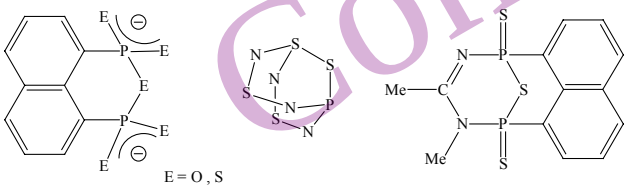
C3e Structural Research Objectives of this YSU / St. Andrews Collaborative Project

C3e(i) Overall Research Objectives: The Woollins group is clearly involved in a variety of interesting synthesis projects. Dr. Slawin and her research group have crystallographically characterized many of their main group derivatives and the two groups have then related this data to their solution phase structures and reactivities. The proposed collaborative research project between Youngstown State University and St. Andrews University will involve high resolution structural studies of selected main group compounds that the Woollins group has prepared. The specific target species are all compounds whose conventional resolution solid state structures have been determined by Dr. Slawin and her group. In each case, these structures differ significantly from what might be expected based on elementary bonding considerations and/or they are at odds with the physical and/or spectroscopic properties in solution and/or the solid state.

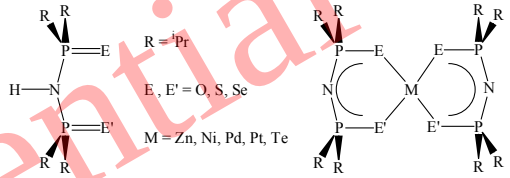
While the specific questions to be answered by each charge density[30] project will vary, they will each proceed using common tools. Over the course of my sabbatical, we plan on developing our skills at using these methods by looking at representative examples from each category of materials. The initial targets will be chosen by balancing their intrinsic scientific importance by the complexity of their structures. Thus, we will start with relatively small and crystallographically well behaved molecules to simplify the complexity of the calculations. We will also chose samples for which the Woollins / Slawin groups already know how to grow the highest quality crystals. Once the PI returns to YSU, this collaboration will continue with more extensive studies of these materials by the collaborators on the two sides of the Atlantic. In particular, the collaborators, and especially the PI, will then be ready to tackle the most scientifically interesting questions even if they present more complex crystallographic and calculation challenges. We plan on the first stage of this crystallographic collaboration taking about 12 - 18 months including the last two thirds of the PI's sabbatical (when all of the data will be collected) as well as additional time back at YSU where some of the calculations and paper writing will be completed.

C3e(ii) Specific Target Molecules: All of these target molecules have been characterized by analytical and spectroscopic means and have had their reactivities explored by the Woollins Group. In addition, conventional resolution diffraction data has been collected and solved by the Slawin group (and in some cases by other groups) on each of these materials (and often on several congeners or a series of closely related materials). We plan on carrying out such studies on about three molecules from each of these 4 groups during this collaborative project. The specific categories from which we plan on beginning our studies over the first year of the collaboration include:

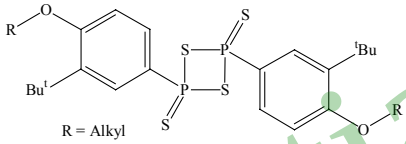
(A) Main Group Rings and Cages[20]



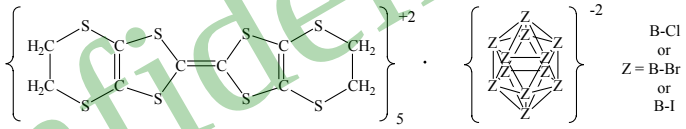
(B) Main Group Ligands and Complexes [21]



(C) Main Group Reagent for Organic Chemistry [23]



(D) Main Group Compounds for Materials Science Applications [24]



By starting this project with a survey of the various classes of Woollins' materials, we will ensure that the PI has the broadest possible experience base for when he returns home (i.e., where he will continue to work on one or more of these categories of main group materials in addition to his own molecules).

C3e(iii) Charge Density Analyses In collaborations with other members of the Woollins / Slawin groups, the structures of each of these complexes will be investigated with an array of complementary techniques to explain their anomalous spectroscopic properties in solution, reactivities, and/or conventional resolution structures in the solid state:

- Using the conventional resolution structures determined by Dr. Slawin's group as our starting point, we will collect high resolution diffraction data for each compound. We will use one of the CCD diffractometers in the Woollins / Slawin Lab to collect the preliminary data using Mo and/or Ag radiation and then the high intensity CLRC Synchrotron at Daresbury to collect the highest resolution data.
- This high resolution data will first be analyzed by conventional methods using SHELXTL[31] and teXsan[32] with which both groups are already familiar. We will then carry out Charge Density analyses on each compound using the method of Coppens.[30a] [Note: The PI will spend several weeks in Philip Coppens' lab at SUNY Buffalo before leaving for St. Andrews to become familiar with the basic operation of this package. Dr. Coppens has agreed to provide additional assistance as necessary both during the sabbatical and after the PI's return to Ohio. The project participants will also be able consult with other crystallographers in southern Scotland who are already carrying out charge density studies.]
- As part of these Charge Density calculations, the participants will carry out space partitioning and topological analysis of the total charge density, calculate the Electrostatic

moments of the charge distribution, calculate the electrostatic potentials, and calculate the electron density and lattice energies of the crystal.

- These results will then be correlated with the results of Molecular Orbital calculations on these compounds to rationalize their bonding and spectroscopic properties.
- Finally, the participants will attempt to use Molecular Mechanics to extend these solid state results to the related molecules in solution.
- Note: Charge Density methods give excellent experimental data on molecular bonding, including the location of the valence electrons in the molecules, the symmetries and topographies of individual bonds, molecular charge distributions, etc. These are used in a synergic fashion with the results of molecular orbital calculations and spectroscopic and physical studies to explain the nature and origins of molecular properties.

Since Drs. Woollins and Slawin have funding for their current research in this area from the UK – EPSRC and industry, see below, we are seeking funding in this NSF International Division grant only to fund the PI's incremental costs of participation in this collaborative research project.

C4 Methodology and Work Plan

During the seven months for which NSF funding for this project is requested (i.e., from December 2000 through June 2001), the PI's efforts will concentrate on several specific objectives for each molecule under study. This project will continue after the PI's return to YSU with data analysis on structures collected in Scotland and additional charge density studies on new molecules.

- The PI is very experienced with growing single crystals.[5,33] Where they are not already available in the lab, the PI will grow crystals suitable for high resolution diffraction analysis. These will be screened for crystal quality using the serial and CCD diffractometers in the Woollins/Slawin lab.
- Good quality diffraction data on these crystals will then be obtained using Mo or Ag radiation on one of the Woollins / Slawin CCD systems at several reduced temperatures. From this data, the motional parameters of the sample will be determined and in many cases the lowest temperature data set will be of sufficiently high quality for the charge density analyses.
- The PI and Dr. Slawin will use the CLRC Synchrotron at Daresbury to collect the high resolution data when this is required (i.e., to take advantage of the short wavelengths and high luminosities available from synchrotrons).
- This high resolution diffraction data will be used to carry out charge density analyses on the compounds from which molecular properties will be calculated as described above.
- The results of these charge density studies will be compared with the results of the Molecular Orbital calculations.
- Finally, the results of these studies will be related to the molecular mechanics studies and the spectroscopic properties in solution and the solid state and the known molecular reactivities.
- The PI's portion of this project will emphasize the diffraction component with other team members playing the lead role in the molecular orbital and molecular mechanics calculations (the spectroscopic and reaction data has already been collected). The high resolution data will be collected on all samples during the PI's sabbatical but some of the data analysis may be completed after his return to Ohio. Indeed, this pattern is likely to be part of the long term collaboration.

C5 Facilities

All requisite facilities to carry out the proposed crystallographic education and research objectives of this project during its term are available at St. Andrews University. The preliminary studies are currently being carried out at Youngstown State University (crystallography education component) and at St. Andrews University (crystallographic research component). These studies will continue to be carried out at both sites after this project is completed but with the addition that more advanced crystallographic research will then be carried out at Youngstown State University (i.e., charge density studies) and St. Andrews University will remain involved in the crystallographic education project as a primary test sites. Details of computer, diffraction, lab, office, etc., facilities of both sites can be found in Section H: Facilities, Equipment, and Other Resources.

C6 Existing Support for the Project

The majority of the costs for this project are being funded from current sources. For example:

- Youngstown State University is providing sabbatical support to the PI for the 2000-2001 academic year ($72,923 total cost for salaries and benefits).
- Youngstown State University is providing some travel funds ($1,600) to the PI to cover half of his return airfare to St. Andrews University as well as to several conferences where the PI is scheduled to give talks on crystallographic education during the summer of 2000.
- Youngstown State University is also providing the PI and his group with no charge access to its instrumentation, including two diffractometers, and computer facilities for this project. It will also provide all requisite materials and reagents that might be needed at YSU before the sabbatical and for the duration of this grant (i.e., to approximately November, 2001).
- Similarly, St. Andrews University and Drs. Woollins and Slawin are also providing the PI with no charge access to its instrumentation, including two CCD diffractometers and "tickets" on the CLRC synchrotron at Daresbury, and computer facilities for this project. Dr. Woollins will also provide all requisite materials and reagents that might be needed at St. Andrews University for this project. The funds for this will come from Drs. Woollins' and Slawin's UK – EPSRC and industrial grants.
- Dr. Woolins is also providing the PI with £6,000 ($9,600) to cover his incremental costs during the first 4 months of his sabbatical at St. Andrews (i.e., for travel, housing, etc.).
- The PI's NSF-DUE-CCLI-EMD-POC grant (#9980921) will cover the US costs of the PI's crystallographic education research project in the US.
- While in Scotland, the PI and his hosts will prepare one or more proposals to UK and US funding agencies (e.g., the EPSRC and NSF) to fund this collaboration over the long term.

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Plenum, NY. (h) W. Jones (Editor), "Organic Molecular Solids: Properties and Applications," **1997**, CRC Press, Boca Raton, FL. (i) C. N. R. Rao, "New Directions in Solid State Chemistry," **1997**, Cambridge University Press, NY. (j) R. C. Buchanan and T. Park, "Materials Crystal Chemistry," **1997**, Marcel Dekker, NY.

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29) (a) C. Hammond, "The Basics of Crystallography and Diffraction (IUCr Texts on Crystallography 3)," **1997**, Oxford University Press, NY. (b) M. F. C. Ladd and R. A. Palmer, "Structure Determination by X-Ray Crystallography," 3rd Edition, **1993**, Plenum Press, NY. (c) G. H. Stout and L. H. Jensen, "X-Ray Structure Determination: A Practical Guide," 2nd Edition, **1989**, Macmillan, NY. (d) For a comprehensive listing of diffraction texts and related materials, see: http://www.as.ysu.edu/~adhunter/Teaching/Chem832/xrayrefs.pdf

30) (a) P. Coppens, "X-Ray Charge Densities and Chemical Bonding (IUCr Texts on Crystallography 4)," **1997**, Oxford University Press, NY. (b) E. Prince and A. J. C. Wilson (Editors), "Advances in the Crystallographic and Microstructural Analysis of Charge Density Wave Modulated Crystals," **1999**, Kluwer, Hingham, MA. (c) P. Coppens, "Synchrotron Radiation Crystallography," **1992**, Harcourt Brace Jovanovich, San Diego. (c) K. Ohno, "Computational Materials Science: from Ab Initio to Monte Carlo Methods," **1999**, Springer, NY. (d) A. Gonis, N. Kioussis, and M. Ciftan (Editors), "Electron Correlations and materials Properties," **1999**, Kluwer, NY.

31) The SHELXTL and XSHELL package of diffraction analysis programs. Available from Bruker-AXS

32) The teXsan package of diffraction analysis programs. Available from Rigaku and Molecular Structure Corporation.

33) (a) A. Hunter's Guide to Growing Single Crystals, see: http://www.as.ysu.edu/~adhunter/Teaching/Chem832/ADHChXIV.pdf (b) A. S. Myerson (Editor), "Molecular Modeling Application in Crystallization," **1999**, Cambridge University Press, NY. (c) C. Reichardt, "Solvents and Solvent Effects in Organic Chemistry," 2nd Edition, **1988**, VCH, NY.

Biographical Sketch for Allen D. Hunter

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a. Professional Preparation:

University of British Columbia, Chemistry	Honors Chemistry	B.Sc.	1981
University of British Columbia, Chemistry	Inorganic Chemistry	Ph.D.	1985
Australian National University, RSC	Organometallic Chemistry	Post. Doc.	1986
University of Alberta, Chemistry	Crystallography	Post. Doc.	1987

b. Appointments:

Youngstown State University, Chemistry	Full Professor	1998-Present
University of Pittsburgh, Crystallography	Visiting Associate Professor	1995-1996
Youngstown State University, Chemistry	Associate Professor	1992-1998
University of Alberta, Chemistry	Adjunct Professor	1992-1995
University of Alberta, Chemistry	Assistant Professor	1987-1992

c. Publications: Allen has a total of 40 peer reviewed publications (22 since 1992) and has also given 36 oral/poster presentations.

(i) Most Closely Related Publications:

1. Smith, C. C.; Jacyno, J. M.; Zeiter, K. K.; Parkanzky, P. D.; Paxson, C. E.; Pekelnicky, P.; Harwood, J. S.; Hunter, A. D.; Lucarelli, V. G.; Lufaso, M. W.; Cutler, H. G.: "Nitration of Cyclopentenecarboxaldehyde: Studies Toward 1-Amino-2-Nitrocyclopentanecarboxylic Acid," *Tetrahedron Letters*, **1998**, *39*, 6617-6620.
2. Cashman, J. R.; Berkman, C. E.; Underliner, G.; Kolly, C. A.; Hunter, A. D.: "Cocaine Benzoyl Thioester: Synthesis, Kinetics of Base Hydrolysis, and Application to the Assay of Cocaine Esterases," *Chem. Res. Toxicol.*, **1998**, *11*, 895-901.
3. Landis, K. G.; Hunter, A. D.; Wagner, T. R.; Curtin, L. S.; Filler, F. L.; Jansen-Varnum, S. A: "The Synthesis and Characterization of Ni, Pd, and Pt Maleonitriledithiolate Complexes: X-Ray Crystal Structures of the Isomorphous Ni, Pd, and Pt ($Ph_2PCH_2CH_2PPh_2$)M(Maleonitriledithiolate) Congeners," *Inorganica Chimica Acta*, **1998**, *282*, 155-162.
4. Hunter, A. D.: "Crystallographic Structure Determination: An Experiment for Organic Analysis and other Non-Traditional Venues," *Journal of Chemical Education*, **1998**, *75*, 1297-1299.
5. Hunter, A. D.: *Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction*, Fall 1998 Version F98D1 © 1997, 1998, 275 pages. Has been released electronically as .pdf files to well over 200 individuals at over 150 Universities around the world. Described in the *Journal of Chemical Education*, **1999**, *76*, 163 and in the ACA and IUCr Newsletters, see: http://www.as.ysu.edu/~adhunter/YSUSC/index.html

(ii) Other Significant Publications:

6. Hunter, A. D.: "A Capstone Writing Experience in Polymer Chemistry: Writing a Proposal to Management for the Purchase of New Polymer Characterization Instrumentation," *Journal of Chemical Education*, **1998**, *75*, 1424.

7. Hunter, A. D.; Bianconi, L. J.; DiMuzio, S. J.; Braho, D. L.: "Synthesis and Structure/Property Relationships in (η^6-Arene)$Cr(CO)_3$ Chemistry: from Guided Experiments to Discovery Research. Physical Properties, IR, MS, and Multinuclear NMR Spectra, and Cyclic Voltammetry," *Journal of Chemical Education*, **1998**, *75*, 891-893.

d. Synergistic Activities:

As can be seen from c4 to c7, above, Allen is very involved in the scholarship of teaching. This has been recognized at YSU by his being designated a Master Teacher in the College of Arts and Sciences, by his recieving substantial Faculty Development Funding for new curriculum innovations, and by his being appointed the Science representative on the General Education Committee, at the state level by his being invited to be a founding member of The Ohio Project for Science Education, and at the national level by several NSF Teaching Instrumentation, Education Materials Development, and Curriculum Innovation grants. He is the representative for Ohio's Predominantly Undergraduate Institutions on the Ohio NMR, MS, and X-Ray Crystallography Consortia. He is on the Advisory Board of the W. M. Keck Foundation Center for Molecular Structure (Cal. State. Fullerton). He is also active in the International Center for Diffraction Data, including its Crystallographic Education subcommittee, in the Council of Undergraduate Research, and he is the organizer of sessions on crystallographic education at upcoming ACA and ACS national meetings. Finally, Allen is very involved with professional development opportunities for regional science teachers.

e. Collaborators & Other Affiliations:

(i) Collaborators:

Bernard Santarsiero, Scripts Institute
Bryan Craven, Indiana University of Pennsylvania and the University of Pittsburgh
Chase Smith, Holly Cross
Derrick Woollins, St. Andrews University
George Richter-Addo, University of Oklahoma
Jim Adrian, Union College
John Cashman, Seattle Biomedical Institute
Mike Zaworotko, University of South Florida
Philip Coppens, University of Buffalo
Simon Bott, University of Houston

(ii) Graduate and Post Doctoral Advisors:

Elliot Burnell (B.Sc.), University of British Columbia
Peter Legzdins (Ph.D.), University of British Columbia
Martin Bennett (Post. Doc.), Australian National University
Martin Cowie (Post. Doc.), University of Alberta
Dietmar Seyferth (Collaborator while a Post. Doc.), M.I.T.

(iii) Thesis and Postgraduate Scholar Sponsor:

X. Andrew Guo, PhD 1994 (University of Alberta), Stan Tsai, PhD 1995 (University of Alberta) Xiaochung Wang, MS 1994 (YSU), Larry J. Bianconi, MS 1994 (YSU), Stanislaus Tsai, PhD 1995 (University of Alberta), Dianne Braho, MS 1995 (YSU), Steven DiMuzio, MS 1996 (YSU), and Bev Smith-Papa, MS 1997 (YSU). ADH has served as the principle advisor for 2 PhD students, 6 MS students, 3 postdoctoral fellows, 3 research associates, and over a dozen undergraduate researchers.

Biographical Sketch for Alexandra M. Slawin

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a. Professional Preparation:

Imperial College	Honors Chemistry	B.Sc.	1983

b. Appointments:

University of St. Andrews	Senior Experimental Officer	1999-Present
University of St. Andrews	Honorary Reader	1999-Present
Loughborough University	Senior Experimental Officer	1994-1999
Imperial College	Experimental Officer	1993-1994
Imperial College	X-Ray Crystallographer	1983-1993

c. Publications: Alex has had over 335 peer reviewed publications (200 since 1992).

(i) Most Closely Related Publications:

1. Synthesis and Structure of platinum(II) complexes with mixed $Ph_2PNHP(O)Ph_2$/[$Ph_2PNHP(O)Ph_2]^-$ or $Ph_2C_6H_4NH_2$/ $[Ph_2C_6H_4NH_2]^-$ hybrid ligands: new M-P-N-H..N-P metallacycles. M. B. Smith and A M Z Slawin, *New. J. Chem.* 2000, 65-67.
2. Reactions of an imidazo[4,5-c]isoxazole-6-carboxylate with electron deficient acetylenes A Taher, A M Z Slawin and G Weaver. *Tetrahedron. Lett*, 1999, **40**, 8157-8162.
3. The synthesis and crystal structures of the first examples of six-membered inorganic iridacycles containing the $[(Ph_2PE)_2N]^-$ ligand (E = S or Se) J Parr, M B Smith and A M Z Slawin, *J.Organomet.Chem.,*1999, **588**, 99-106.
4. Crystallisation of H_3BTC, H_3TPO or H_2SDA with M^{II} (M = Co, Mn or Zn) and 2,2'-bipyridyl: design and control of co-ordination architecture, and magnetic properties (H_3BTC =benzene-1,3,5-tricarboxylic acid, H_3TPO = tris(4-carboxylphenyl)phosphine oxide, H_2SDA = cis-stilbene-4,4'-dicarboxylic acid) M J Plater, M S J Foreman, E Coronado, C J Gomez Garcia and A M Z Slawin, *JCS Dalton*, 1999, 4209-4216.
5. Chiral oxime ethers in asymmetric synthesis. Part 4. Asymmetric synthesis of N-protected amines and beta-amino acids by the addition of organometallic reagents to ROPHy/SOPHy-derived aldoximes J C A Hunt, C Lloyd, C J Moody, A M Z Slawin and A K Takle, *JCS Perkin.* 1, 1999, 3443-3454.

(ii) Other Significant Publications:

6. Preparation of a range of copper complexes of diphenylsulfimide: X-ray crystal structures of $[Cu(Ph_2SNH)_4]Cl_2$ and $[Cu_4O)(Cl)_6(Ph_2SNH)_4]$ P. F. Kelly PF, S M Man, A M Z Slawin K.W Waring, *Polyhedron,* 1999, **18**, 3173-3179.
7. Novel bimetallic lead(II) complexes of polydentate amine-phenol ligands. P. Bhattacharyya, J. Parr and A.M.Z. Slawin, *Inorg. Chem. Commun.*1999, **2**, 113-115.
8. Coordination networks with 1,3-bis(4-pyridyl)propane. A flexible ligand exhibiting supramolecular isomerism M.J. Plater, M.R.S Foreman and A.M.Z Slawin, *J. Chem. Res.-S*, 1999, 74-75A.
9. "Smart" rotaxanes: Shape memory and control in tertiary amide peptido[2]rotaxanes. W. Clegg, C. Gimenez-Saiz, D. A. Leigh, A. Murphy, A.M.Z. Slawin and S.J. Teat, *J. Am. Chem. Soc.*1999, **121**, 4124-4129.
10. Chiral oxime ethers in asymmetric synthesis. 3. Asymmetric synthesis of (R)-N-protected alpha-amino acids by the addition of organometallic reagents to the ROPHy oxime of

cinnamaldehyde C. J. Moody, P. T. Gallagher, A.P. Lightfoot and A.M.Z. Slawin, *J. Org. Chem.,* 1999, **64**, 4419-4425.

d. Synergistic Activities:

Alex's main research interests lay in the area of diffraction analysis. She is an expert is both serial and area detector equipped lab diffractometers and in using synchrotron systems to collect high resolution diffraction data. Many of these studies are done in collaboration with synthetic chemists. In addition, she maintains an active research program in the area of supramolecular chemistry.

e. Collaborators & Other Affiliations:

(i) Collaborators:

Prof D A Leigh, University of Warwick.

(ii) Graduate and Post Doctoral Advisors:

Prof D J Williams, Imperial College London

(iii) Thesis and Postgraduate Scholar Sponsor:

PDF Carlos Gimenez Saiz.

Biographical Sketch for J. Derek Woollins

Department of Chemistry, St. Andrews University, St. Andrews, Fife, KY16 9ST, Scotland
44-01334-463861, J.D.Woollins@st-and.ac.uk,
http://ch-www.st-and.ac.uk/staff/jdw/index.html

a. Professional Preparation:

University of East Anglia	Honors Chemistry	B.Sc.	1976
University of East Anglia	Inorganic Chemistry	Ph.D.	1979
University of British Columbia	Organometallic Chemistry	Post. Doc.	1979-80
Michigan State University	Inorganic Chemistry	Post. Doc.	1980-81
University of Leeds	Inorganic Chemistry	Post. Doc.	1983-84

b. Appointments:

St. Andrews University	Professor of Synthetic Chemistry	1999-Present
Loughborough University	Professor of Inorganic Chemistry	1994-1999
University of London	Reader	1990-1993
University of London	Recognized Teacher	1986-1989
Imperial College	Lecturer	1984-1985
Michigan State University	Assistant Professor	1981-1983

c. Publications: Derek has had over 239 peer reviewed publications (140 since 1992).

(i) Most Closely Related Publications:

1. Synthesis and X-Ray Crystal Structures of Tellurium Complexes Containing Imidophosphinate Ligands. D. J. Birdsall, J. Novosad, A. M. Z. Slawin and J. D. Woollins, *J. C. S. Dalton. Trans.,* 2000, 435-439.
2. A Novel Alanine Derivatised Phosphine. Alexandra M. Z. Slawin, J. Derek Woollins and Qingzhi Zhang, *Inorg Chem. Comm*. 1999, **2**, 386-8.
3. Reactions of dithiadiphosphetane disulfides with organonitrogen compounds. M. R. St. J. Foreman, R. J. Mortimer, A. M. Z. Slawin and J. D. Woollins. *J. Chem. Soc., Dalton Trans.* 1999, 3419-3430.
4. The preparation of a solubilised form of Lawessons Reagent and its thionation reactions. M. R. St. J. Foreman, A. M. Z. Slawin and J. D. Woollins. *Heteroatom Chem*. 1999, **10**, 651-657
5. Novel condensed thionated bis(phosphonic) acid salts with a rigid naphthalene-1,8-diyl backbone. P. Kiliàn, A. M. Z. Slawin and J. D. Woollins. *Eur. J. Inorg. Chem*. 1999, 2327-2333.

(ii) Other Significant Publications:

6. Phosphino-urea chemistry: Preparation and structure of chelate and P-N Bond Cleavage Complexes. A. M. Z. Slawin, M. Wainwright and J. D. Woollins, *New J Chem.* 2000, **24**,69 - 72.
7. New P-S-N containing ring systems. Reaction of 2,4-(naphthalene-1,8-diyl)-1,3,2,4-dithiadiphosphetane-2,4-disulfide with N, N-bis(trimethylsilyl)methylamine. Petr Kilián, Jaromír Marek, Radek Marek, Jaromír Tousek, Otakar Humpa, Alexandra M. Z. Slawin, Jirí Touzín, Josef Novosad and J. Derek Woollins, *J. Chem. Soc., Dalton Trans.* 1999, 2231-2236.
8. Displacement of triphenylphosphine from $Cu(PPh_3)_2NO_3$ and $Co(PPh_3)_2Cl_2$ by a diselenoimidodiphosphinato ligand. X-ray crystal structure of $(PPh_3)Cu[Ph_2P(Se)NP(Se)Ph_2]$ and $Co[Ph_2P(Se)NP(Se)Ph_2]_2$ containing the novel

$CuSe_2P_2N$ and $CoSe_2P_2N$ inorganic metallacycles. J. Novosad, M. Necas, J. Marek, P. Veltsistas, C. Papadimitriou, I. Haiduc, M. Watanabe and J. D. Woollins, *Inorg. Chim. Acta*, 1999, **290**, 256-260.

9. Synthesis and X-ray Crystal Structure of $[CuN(R_2PS)_2]_3$, David J. Birdsall, Alexandra M. Z. Slawin and J. Derek Woollins. *Inorg. Chem*. 1999, **38**, 4152-4154.
10. Reaction of Large-bite Ligands with Various Tellurium Compounds. Synthesis and Structural Characterization of $[Te(\mu\text{-}Cl)_2\{(SPPh_2)_2N\}_2]$, $[(4\text{-}MeOC_6H_4TeCl_3)_2\{\mu\text{-}Ph_2P(S)CH_2CH_2P(S)Ph_2\}]$ and $[Te_2(\mu\text{-}S_2PPh_2)_2]$ Representing Novel Types of Tellurium Complexes, J. Novosad, K. W. Törnroos, M. Necas, A. M. Z. Slawin, J. D. Woollins and S. Husebye. *Polyhedron* 1999, **18**,2861-2867.

d. Synergistic Activities:

Derek has collaborated and consulted extensively with industry, including with EXXON Chemicals, Abingdon, and Inorgtech. He is Inorganic Textbook series editor for John Wiley and for the Royal Society's Tutorial Texts series. He is the UK editor of *Main Group Chemistry* and is chair of the editorial board of *Chemistry in Britain*. He is very active in undergraduate and graduate education and in the mentoring of new faculty. His research group is active in a wide range of areas related to the synthesis and characterization of main group inorganic and organometallic ring systems. He is also interested in their use organic reagents and as ligands for transition metal complexes and as catalysts and/or co-catalysts.

e. Collaborators & Other Affiliations:

(i) Collaborators:

Prof Ralf Steudel, Technical University, Berlin.
Prof D J Williams, Imperial College London
US FILTER, Illnois.

(ii) Graduate and Post Doctoral Advisors:

PhD: Prof A J Thomson, University of East Anglia, Norwich
PDF: Prof W R Cullen, Dept of Chemistry UBC, Vancouver
Prof B Rosennberg, Michigan State, East Lansing Michigan
Prof N N Greenwood, Leeds, UK

(iii) Thesis and Postgraduate Scholar Sponsor:

PhD: D J Birdsall 1999; S M Aucott 1999; R Reynolds 1999; M Forema 1998; T Q Ly 1998; J Phillips 1997; R Keyte 1997; C Denekamp 1995; C Wong 1995; P Bhattacharyya 1994; V Ginn 1992; M Pilkington 1993; J C Fitzmaurice 1990

PDF: Maria Parr; N Smith, J Green; P Kilian; M B Smith; P Bhattacharyya.

SUMMARY PROPOSAL BUDGET

YEAR 1

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **Youngstown State University**

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Allen D Hunter**

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2.					
3.					
4.					
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**1**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**0**	
2. FOREIGN				**3,700**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**11,760**	
TOTAL OTHER DIRECT COSTS				**11,760**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**15,460**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **(Rate: , Base:)**					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**15,460**	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **15,460**	$

M. COST SHARING PROPOSED LEVEL $ **84,123** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*: **Allen D Hunter** DATE

ORG. REP. TYPED NAME & SIGNATURE* DATE

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET

Cumulative

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **Youngstown State University**

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Allen D Hunter**

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**1**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**0**	
2. FOREIGN				**3,700**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**11,760**	
TOTAL OTHER DIRECT COSTS				**11,760**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**15,460**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**15,460**	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **15,460**	$

M. COST SHARING PROPOSED LEVEL $ **84,123** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*: **Allen D Hunter** DATE

ORG. REP. TYPED NAME & SIGNATURE* DATE

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

NSF Form 1030 (10/99) Supersedes all previous editions

C***SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPG III.B)**

Section F: Budget Justification

Line E2, Foreign Travel:

The requested funds on this international travel budget line total $3,700. Of this request, $400 is to cover half of the cost of a round trip economy air fare from Pittsburgh (the nearest international airport to Youngstown) to Edinburgh and ground transportation from Youngstown to Pittsburgh (≈50 miles) and from Edinburgh to St. Andrews (≈50 miles) for the PI (i.e., leaving approximately August 1st, 2000 and returning in mid July, 2001). Travel from St. Andrews to the CLRC synchrotron source at Daresbury (approximately once a month) to collect high resolution diffraction data will lead to $2,800 in incremental expenses. The return train fair from St. Andrews to Daresbury is approximately $70, accommodations will be approximately $70 per night, and meals/incidentals will be approximately $30 per day (i.e., $400 for 3 night/4 day visits). I also request funds totaling $500 to attend the 2001 British Crystallographic Association annual meeting (April 7th-10th of 2001 at Reading University) to present the results of my collaborative research projects.

Line G6, Other Direct Costs; Other:

This budget item of $11,280 for other direct costs is to cover the incremental expenses for seven months. The PI has found a furnished apartment in St. Andrews for £800 per month (i.e., $1,280) and will rent/lease a mid-size car/van for approximately $400 per month. [Note: Because of her seizure disorder, the PI's daughter requires a wheel chair to move around. A letter from her physician stating this and explaining her condition can be supplied on request. The PI will therefore require both a wheel chair accessible apartment and appropriate vehicle.] Utilities, council fees, gasoline, food, clothing, laundry, etc., costs will total at least $1,800 per month. The total projected costs are therefore approximately $3,480 per month. Of these costs, approximately $1,800 would be incurred if the PI stayed in Youngstown for the sabbatical. The PI therefore requests $1,680 per month for incremental expenses (i.e., for 7 months the NSF request totals $11,760, i.e., from December 1st, 2000 to June 30th, 2001).

Line M, Cost Sharing; Proposed Level:

Youngstown State University is providing the PI with full salary and benefits during his sabbatical at St. Andrews with a total value of $72,923 (i.e., $55,250 for salary and $11,787 for benefits (at 32%)). Of this amount, 1/3 is currently committed to the educational methods research portion of this collaborative project (i.e., $24,303). The remaining 2/3, valued at $48,620 is provided as a salary and benefits match to the research component of this current proposal. In addition, YSU is providing the PI with $1,600 towards travel costs during the period of the sabbatical (these funds will be used to pay for half of the PI's travel costs to St. Andrews and partially offset the costs of attending diffraction methods conferences in the UK and Europe during the first 4 months of his sabbatical). Dr. Woollins has also committed £6,000 from his UK – EPSRC grants (i.e., $9,600) towards the PI's incremental costs during the first four months of this collaborative project. Thus, the total salary, benefits, travel, and incremental costs match to this collaborative project is approximately $84,123. If the NSF prefers to consider only the crystallographic research component of this match, it totals approximately $48,620. Both St. Andrews and YSU will also provide reagents, cryogens, facilities, diffractometer and computer time. The estimated value for these is approximately $30,000 but they are not included in the formal match.

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information

Investigator: **Allen D. Hunter** | Other agencies (including NSF) to which this proposal has been/will be

Support: ■ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: X-Ray Diffraction Analysis Throughout the Curriculum: a Powerful Tool for Understanding Molecular Structure and Bonding

Source of Support: NSF-DUE-CCLI-EMD-POC # 9980921

Total Award Amount: $74,707 Total Award Period Covered: 05/01/2000 – 04/30/2002

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: 3 Sumr: 1

Support: ■ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: The Ohio Project for Science Teaching

Source of Support: Ohio Board of Regents

Total Award Amount: $4,000 to YSU Total Award Period Covered: 07/01/1999 – 06/30/2000

Location of Project: Youngstown State University and other Ohio Universities

Person-Months Per Year Committed to the Project. Cal: 0.5 Acad: Sumr:

Support: ■ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: A Proposal to Establish a State-of-the-Art Ohio Mass Spectrometry Consortium

Source of Support: Ohio Board of Regents Investment Fund

Total Award Amount: $88,900 to YSU Total Award Period Covered: 06/01/1999 – 05/31/2000

Location of Project: Youngstown State University and other Ohio Universities

Person-Months Per Year Committed to the Project. Cal: 0.5 Acad: Sumr:

Support: ■ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Investigative Approaches in the Natural Sciences

Source of Support: NSF-DUE-IWR #9850079

Total Award Amount: $183,579 Total Award Period Covered: 06/01/1998 – 05/31/2001

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

Support: ■ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment

Source of Support: NSF-DUE-ILI #9851107

Total Award Amount: $44,600 Total Award Period Covered: 06/01/1998 – 05/31/2001

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: 3 Acad: Sumr:

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*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information

Investigator: **Allen D. Hunter** (continued)	Other agencies (including NSF) to which this proposal has been/will be

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: A Proposal for Fulfilling the Goals of the Oho Mass Spectrometry Consortium

Source of Support: Ohio Board of Regents Investment Fund
Total Award Amount: $106,000 to YSU Total Award Period Covered: 06/01/2000 – 05/31/2001
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 0.2

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this

Investigator: **Alexandra Slawin**

Other agencies (including NSF) to which this proposal has been/will

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Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: P-N Bond Forming Reaction for the Synthesis of New Multifunctional P(III) and P(V) Species

Source of Support: UK – EPSRC Grant

Total Award Amount: £ 227,159 Total Award Period Covered: 11/01/1999 – 10/31/2002

Location of Project: St. Andrews University

Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CCD System for X-Ray Crystallography

Source of Support: UK - EPSRC

Total Award Amount: £ 75,000 Total Award Period Covered: 03/01/97 – 02/28/2001

Location of Project: St. Andrews University

Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Cal: Acad: Sumr:

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*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this

Investigator: **J. Derek Woollins** | Other agencies (including NSF) to which this proposal has been/will

Support: ◙ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: P-N Bond Forming Reaction for the Synthesis of New Multifunctional P(III) and P(V) Species

Source of Support: UK – EPSRC Grant
Total Award Amount: £ 227,159 Total Award Period Covered: 11/01/1999 – 10/31/2002
Location of Project: St. Andrews University
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ◙ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Metathesis Reactions for the Synthesis of Inorganic Rings and Cages

Source of Support: UK - EPSRC
Total Award Amount: £ 151,514 Total Award Period Covered: 10/01/1998 – 09/30/2001
Location of Project: St. Andrews University
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ◙ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: P-S and P-Se Chemistry:
Investigation into the Identity of Woollins Reagent:
The Synthesis of New Binary Systems
Source of Support: UK - EPSRC
Total Award Amount: £ 145,884 Total Award Period Covered: 09/01/1998 – 08/31/2001
Location of Project: St. Andrews University
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ◙ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: CCD System for X-Ray Crystallography

Source of Support: UK - EPSRC
Total Award Amount: £ 75,000 Total Award Period Covered: 03/01/97 – 02/28/2001
Location of Project: St. Andrews University
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ◙ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Modernization & Development of Microanalytical Facility for Synthesis Program at St. Andrews

Source of Support: UK – EPSRC and Zeneca
Total Award Amount: £ 42,000 Total Award Period Covered: 03/01/2000 – 02/28/2003
Location of Project:
Person-Months Per Year Committed to the Cal: Acad: Sumr:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this

Investigator: **J. Derek Woollins** (continued)	Other agencies (including NSF) to which this proposal has been/will

Support: ◙ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Oxidation Chemistry of H2S

Source of Support: US Filter
Total Award Amount: £ 51,000 Total Award Period Covered: 10/01/1999 – 09/30/2001
Location of Project: St. Andrews University
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: Acad: Sumr:

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*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Section H: Facilities, Equipment, and Other Resources

Laboratory Facilities: At both YSU and St. Andrews, the PI will have access to modern laboratory facilities. At St. Andrews, the Chemistry department is housed in the Purdie Building, which offers excellent facilities for visiting researchers. The PI will perform any required "wet chemistry" (especially crystal growing activities) in one of Dr. Woollin's research labs. Smaller items of equipment, such as HPLCs and IR, UV-visible, and NMR spectrometers are housed in adjacent equipment rooms to which the PI will have full access. At YSU, the PI also has his own "wet chemistry" research space and access to appropriate instrumentation and spectrometers. The PI will also be assigned office space in the Purdie Chemistry Building near the other members of the Woollins / Slawin groups.

Computer Facilities: Dr. Woollins' and Dr. Slawin's research groups are both equipped with well developed personal computer facilities supported by laser printers which will be made available to the PI. The PI will have access to more advanced computers on site, including: Floating Point Systems supercomputers, DEC VAX workstations, and over twenty Silicon Graphics (most with R4000 processors), SUN, and Tektronics workstations for high resolution molecular graphics and fast diffraction analysis, molecular mechanics, and dynamics calculations. At YSU, the PI has several personal computers (including: a Windows NT and a Windows 98 PC, a SGI Indy workstation, and both color and laser printers), access to excellent departmental computer labs (including dozens of Windows PCs and 6 SUN and SGI workstations), and access to the Ohio Super Computer Center (if this is needed).

Youngstown State University Structure Center: The YSU Structure Center, which has the PI as its director, is very well equipped for a PUI. For example, it includes the following research grade equipment (which is all 6 years old or younger): a Varian 400 MHz multinuclear NMR equipped with 4 probes, PFG, and VT, two GC-MS system and one LC-MS (APCI and ESI), thermal analysis equipment (a DSC and a TGA), Viscometry equipment, a GPC (with autosampler and diode array UV-Vis., and RI detectors), as well as many other chromatographic, analytical, and spectroscopic instruments. Most relevant to this proposal, the Structure Center is equipped with two Bruker-AXS diffractometers, one with a LT2 low temperature system and one with a X-1000 multiwire area detector. All of this instrumentation is available to the PI and his students (and indeed faculty and students from other PUIs) at no charge.

St. Andrews University Diffraction Facilities: St. Andrews Universities is equipped with a complete array of the most modern diffraction facilities, including: cutting edge instrumentation for powder, macromolecular, and small molecule crystallography. For example, in addition to departmental instrumentation and that in the other 4 crystallography research groups, the Woollins and Slawin groups have several conventional diffractometers equipped with serial detectors as well as two new CCD systems (one from Bruker-AXS and one from Rigaku-MSC). The PI will have complete access to these instruments as well as to any other characterization facilities he needs (e.g., St. Andrew's has half a dozen multinuclear NMRs including a 500 MHz solid state system and two 500 MHz solution phase instruments) at no charge. In addition, these groups routinely collect high resolution synchrotron diffraction data at the CLRC Daresbury laboratory. Through is collaborations with them, the PI will have access to this facility as needed for his project. St. Andrews is equipped with the full range of support staff and facilities expected of a major research university and the PI will have access to all of these as appropriate for his collaborative project.

CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

(1) the statements herein (excluding scientific hypotheses and scientific opinions) are true and complete, and
(2) the text and graphics herein as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or individuals working under their supervision. I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this proposal.

I understand that the willful provision of false information or concealing a material fact in this proposal or any other communication submitted to NSF is a criminal offense (U.S.Code, Title 18, Section 1001).

Name (Typed)	Signature	Social Security No.*	Date
PI/PD **Allen D Hunter**		SSNs are confidential and are not displayed *ON FASTLANE SUBMISSIONS*	
Co-PI/PD			
Co-PI/PD			
Co-PI/PD			
Co-PI/PD			

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding Federal debt status, debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in Grant Proposal Guide (GPG), NSF 00-2. Willful provision of false information in this application and its supporting documents or in reports required under an ensuring award is a criminal offense (U. S. Code, Title 18, Section 1001).

In addition, if the applicant institution employs more than fifty persons, the authorized official of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of Grant Policy Manual Section 510; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflict which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF.

Debt and Debarment Certifications

(If answer "yes" to either, please provide explanation.)

Is the organization delinquent on any Federal debt? Yes ☐ No ☒

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency? Yes ☐ No ☒

Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding $100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding $150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

(1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.

(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME/TITLE (TYPED) **Dr. Peter J. Kasvinsky/Graduate Dean**		**04/25/00**

TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS	FAX NUMBER
330-742-3091	**amgrad03@ysub.ysu.edu**	**330-742-1580**

*SUBMISSION OF SOCIAL SECURITY NUMBERS IS VOLUNTARY AND WILL NOT AFFECT THE ORGANIZATION'S ELIGIBILITY FOR AN AWARD. HOWEVER, THEY ARE AN INTEGRAL PART OF THE INFORMATION SYSTEM AND ASSIST IN PROCESSING THE PROPOSAL. SSN SOLICITED UNDER NSF ACT OF 1950, AS AMENDED.

Certification of RUI Eligibility

CERTIFICATION OF RUI ELIGIBILITY

[This certification, executed by an Authorized Institutional Representative, should appear as Page 1 of Proposal Section I (i.e., as Page I-1).]

By submission of this proposal, the institution hereby certifies, as evidenced by the signature below, that the proposal is from a department that offers courses leading to a bachelor's or master's degree, but does not offer a doctorate, or doctoral courses and the supervision of doctoral research, and is located on a campus where the total number of doctorates awarded in fields supported by NSF did not exceed 20 in the two academic years preceding the proposal submission.

AUTHORIZED INSTITUTIONAL REPRESENTATIVE

Dr. Peter Kasvinsky
Dean of Graduate Studies and Research

Signature

Date 4/27/00

RUI Impact Statement

The Situation at Predominantly Undergraduate Institutions, PUIs: PUIs have significantly different emphases in their missions than do PhD granting research universities. In general, their mission is more heavily focussed on undergraduate students and less on externally funded research. In many cases, PUIs also have a greater level of support / encouragement for the scholarship of teaching. This difference in missions is reflected in many areas, including: teaching loads that are typically much higher than at larger universities, smaller class sizes with fewer advanced offerings, and an emphasis on undergraduates as the primary research personnel. In addition, the trend across the country at PUIs is get all undergraduates involved in research like laboratory experiences and in publishable research projects. This research involvement is extremely beneficial to the students but it is also very time consuming for the faculty. This combination of factors has been widely recognized to lower the productivity of undergraduate faculty *in terms of publication rate.* However, it does have a more positive side in that it does tend to allow/encourage: a greater degree of one on one interactions with undergraduates, more experimentation with novel approaches to teaching, more interest in the scholarship of teaching, and more emphasis on the integration of teaching and research.

Youngstown State University as a PUI: Youngstown State University is an urban PUI situated in the heart of downtown Youngstown. It has approximately 12,000 undergraduates enrolled in 1 and 2 year associate degrees (more commonly found at community colleges) and in 4 year bachelors degrees from our Colleges of Arts & Sciences, Business, Education, Engineering, Fine & Performing Arts, and Health & Human Services. We also have a variety of MS level programs totaling approximately 1,200 students (primarily in the college of education) but offer no PhDs in NSF supported fields. YSU is an *open enrollment commuter institution* (more than 90% of our students live off campus). Reflecting our region's blue collar roots, the typical YSU student is in the first generation of their family to attend college and works an average of 30 hours per week to support their studies. Our students are a relatively hard working and motivated group, but this combination of factors significantly impacts our ability to get them involved in research.

Encouraging Undergraduates to Participate in Research: To encourage a greater research participation by all students, our new General Education program (on which committee the PI serves) has been restructured and it will be implemented in the Fall of 2000. One aspect of this change has been to very strongly encourage all lab (and to the extent possible, lecture) courses to follow a *discovery oriented collaborative research model.* This is facilitated by the small size of our upper level labs and courses (i.e., 5 to 25 students). In addition, many science labs are being restructured to integrate research like (or even real research) projects with the more skills oriented exercises. Finally, we are now going to require all bachelors students to complete a capstone course which integrates research, written and oral communication, and critical thinking components. In the sciences, this course will typically be a undergraduate research project coupled to a course that gives formal training in these areas.

The Research Situation in the YSU Chemistry Department: Our department is considered one of the strongest, if not the strongest, on campus and the administration holds us up as the model of how to integrate scholarship, teaching, and service in a synergic fashion. We

have 15 full time faculty positions divided between our Biochemistry, Analytical, Inorganic, Organic, and Physical Divisions and our new Chemical Education Division. Each division is similar in size with many faculty being associated with more than one division. For example, the PI teaches largely in the Organic Division but also covers some Biochemistry and Inorganic Courses and his research interests span the range of organometallic and polymer chemistry, diffraction methods, and Chemical Education.

Recent Changes in the YSU Chemistry Department: 10 of our 15 faculty have been at YSU for 8 years or less. This, coupled with the strong support of the senior and retired faculty and a total replacement of the administration, has enabled a dramatic change in our department's activities and profile. A decade ago, the scale of externally funded research in our department was limited (largely due to administrative impediments) and was concentrated in the Analytical and Physical Divisions. With our rejuvenation, almost all faculty are now involved in research. Both our publication rates and our success at raising external funding to support this effort have increased dramatically (e.g., by more than an order of magnitude for external grants). The PI and the Department have been particularly successful in funding state of the art instrumentation for use in our courses and student research projects.

The Chemistry Program at YSU: Our department graduates approximately 30 – 40 BA and BS majors in Chemistry and 5 –10 MS students each year. Our students have developed an *extremely strong regional and growing national reputation* for the quality of their preparation for either graduate school or industry. As part of our new General Education program, and reflecting the simultaneous change from quarters to semesters, we have fundamentally revised our undergraduate and MS course sequences. For example, our BA and ACS approved BS students will now complete all of their required courses in their first three years. This will leave their Senior year free to be focussed on research like laboratory courses, undergraduate research projects, and (for many) internship experiences. This should significantly enhance the integration of their teaching and research experiences and the extent of their evolvement in research. We have decreased the formal course load which our MS students are required to take and rearranged our offerings so that the students will be able to complete them in their first year (rather than the 5 quarters typical now). We have also instituted more formal training in chemical safety, research, writing, and presentations. Again, this combination should significantly increase their research productivity. Finally, we have always had several less formal programs to support the professional development needs of regional teachers. We are now instituting more formal programs, including: a new College of Arts and Sciences/College of Education program for pre-service teachers and new masters level programs for in-service teachers. The masters programs will include an MS in Chemistry with a Chemical Education Emphasis (Fall 2000 start) and an MA in Science Education. The MS in Chemistry will require the same core chemistry courses as our other MS programs but will differ in that the research project will be in the area of Chemical Education.

The Research Facilities at YSU: The PI came to YSU 8 years ago from a PhD institution where his research had focussed on Organometallic and Polymer Chemistry. When he arrived at YSU there was a very supportive environment towards research but almost no appropriate equipment or instrumentation for modern synthetic research. Since that time, he and a group of collaborators, some from other departments at YSU or from regional colleges, have

worked diligently to build the infrastructure at YSU so as to be able to do competitive research. This infrastructure is now largely in place. For example, YSU now has the following modern instrumentation: a 400 MHz multinuclear NMR spectrometer equipped with PFG and VT, an LC-MS and two GC-MS systems, Thermal Analysis and GPC instrumentation for Polymers, a variety of other chromatography, analytical, and spectroscopic instrumentation, and two P4 single crystal diffractometers including a multi-wire area detector and a LT2 system. The department is now helping plan a new science building for 2007.

The PI's Scholarly Program at YSU: For his first several years at YSU, the PI maintained an emphasis in his scholarship on the synthetic chemistry of organometallic compounds and polymers. However, this program was hard to carry out in the absence of appropriate characterization instrumentation, he therefore directed his grant seeking activities to acquiring research grade instrumentation for use in student research and teaching. This activity has now begun to slow because most of the required items are now in place. Through a combination of encouragement from his administration, the interests of his students, and changing interests, the PI then became increasingly involved in the scholarship of teaching. Indeed, he currently has the large majority of his scholarly activities in this area. However, he strongly believes that he has moved too far in this direction and would like to re-energize his research program, to take better advantage of the synergies between teaching and research ,and to reenter the research mainstream. He therefore planned the sabbatical described in this proposal that includes components of both types of scholarly activity but with an emphasis on crystallographic research.

Benefits to the PI, YSU, and Other US Colleges, from the Proposed Project: At the completion of this project, the PI will have updated his knowledge base and improved his skills in several different areas, including:

(a) Diffraction Teaching Materials for Undergraduates

The first 4 month phase of this collaborative research project will emphasize the development and revisions of crystallographic education materials aimed primarily at undergraduates. These materials will be tested at St. Andrews as well as US sites to ensure that they meet the broadest range of student needs. These materials will directly benefit large numbers of students at YSU and other US Colleges who will use them in their undergraduate classes. If the PI were not to have the sabbatical time available, this project would certainly proceed much more slowly and with less varied feed back.

(b) Main Group Inorganic Chemistry

The PI has had very little exposure to main group inorganic chemistry since his class work as an undergraduate and some research on phosphine synthesis as a postdoctoral fellow in Australia. While it is possible to teach on topics about which one has little or no practical experience, such efforts lack the intrinsic excitement and personal experience that enriches coursework where one has practical expertise. Both from learning some aspects of main group chemistry for the collaborative research project and being a member of a main group inorganic research team (and hence participating in both the formal and informal group discussions), the PI will be able to infuse his teaching on topics related to main group chemistry back at YSU with new vitality. For example, this will allow the insertion of new materials and experiences on main group chemistry into the PI's Inorganic, Organic, and Instrumental Methods courses.

(c) The Use of X-Ray Area Detectors Including: CCD and Imaging Plate Systems

While the PI has used area detectors several times over the last 3 years and teaches about the theory of their use now, he does not have enough skill in their use to operate them independently of other crystallographers or to discuss the practical aspects of their use in his classes and teaching materials. The skills and familiarity gained over the course of this sabbatical project will enable the PI to include information on their use in his teaching materials and classes and will enable he and his undergraduate research students to use such systems (which are available at several universities within 4 hours drive) to collect data for their research.

(d) The Use of Synchrotron Sources to Collect Diffraction Data

The PI has no experience with using synchrotron sources only teaches the very basics of their use now. He certainly does not have enough experience to even have a gut level understanding of their strengths and weaknesses or to discuss the practical aspects of their use in his classes and teaching materials. The skills and familiarity gained over the course of this sabbatical project at the CLRC synchrotron at Daresbury will enable the PI to include information on their use in his teaching materials and classes. It will also facilitate his and his undergraduate research students use of such systems (which are available to PUI faculty and students at national labs) to collect data (with the assistance of the operator) for their research.

(e) Charge Density Diffraction Analysis Methods

The PI is just beginning to learn charge density methods. He will gain some basic familiarity with them this summer at SUNY Buffalo and then intensively concentrate on learning them during his sabbatical. This will both feed back into his teaching materials and classes, but, more importantly will prepare him to start using them in his research. Charge density methods are now becoming accessible for joint faculty/undergraduate student research projects and the PI plans on making these the central focus of his scholarly activity when he returns to YSU.

(f) Molecular Orbital and Mechanics Calculations

The PI will assist the individuals doing these calculations as part of the collaboration and will gain enough experience to discuss them with increased familiarity in his classes. Over the following several years he hopes on increasing his skills with this type of calculations to support his and his students charge density studies.

(g) Long Term Collaboration

One of the primary benefits of this project will be the establishment of a long term collaboration on both the scholarship of crystallographic education and research between the PI at YSU and Drs. Woollins and Slawin at St. Andrews University. Such productive collaborations are vital to maintaining a productive research program at a Predominantly Undergraduate Institution. These individuals plan on writing proposals to conventional NSF and EPSRC program during the term of this grant to fund this collaboration in the future.

DIVISION OF INTERNATIONAL PROGRAMS COVER PAGE

Country: ___Scotland (UK)_____

Field of Science or Engineering: ___Chemistry_____

Proposal Category:

[*] Cooperative Research

[ ] Joint Seminar or Workshop

[ ] Planning Visit

[ ] Dissertation Enhancement

[ ] International Research Fellow awards: Use Cover Sheet in Appendix IV

Foreign Counterpart Investigator/Organizer

Name: __Professor. Derek Woollins_____

Department: __Chemistry_____

Institution: ____St. Andrew's University_____

Address: ___The Purdie Building, The University, St. Andrews,_____

___Fife, KY16 9ST, Scotland_____

Telephone: ____Ph. 44-1334-463861____ FAX. 44-1334-463384_____

Fax or electronic mail (if known): __ j.d.woollins@st-andrews.ac.uk __

For Joint Seminar or Workshop

Location: _____

Date(s): _____

Is the proposed meeting related to any other held or scheduled within one year?

_____

If so, provide name and site of other meeting: _____

J Derek Woollins
Tel 44-1334-463861
Fax 44-1334-463384
Email j.d.woollins@st-andrews.ac.uk

SCHOOL OF CHEMISTRY,
THE PURDIE BUILDING,
THE UNIVERSITY,
ST. ANDREWS,
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SCOTLAND

UNIVERSITY OF ST. ANDREWS

Dr. Rose Gombay
Program Officer for Scotland and the UK
Division of International Programs
Directorate of Social, Behavioral, and Economic Sciences
National Science Foundation
4201 Wilson Blvd
Arlington, VA 22230

April 19th, 2000

Dear Dr. Gombay

With this letter, I would like to confirm that Dr. Allen D. Hunter of the Youngstown State University Department of Chemistry is invited to spend his 2000-2001 sabbatical at our university. They University of St. Andrew's crystallography group includes a critical mass of faculty and staff (including Drs. Slawin, Woollins, Naismith, Taylor, and Bruce) with expertise in almost all areas of modern crystallography. My lab is especially well equipped to carry out cutting edge crystallographic research being equipped with a range of modern diffractometers (including two instruments with CCD detectors) as well as access to the CLRC synchrotron source at Daresbury. We are offering Dr. Hunter access to all of our instrumentation and facilities while he is here. I have been in contact with Dr. Hunter for several years. Initially, this interaction grew out of our joint interest in the teaching of diffraction methods – we use Dr. Hunters current lab manual for this purpose. More recently, we have begun to outline a joint research project as well.

The collaboration between myself and other St. Andrew's faculty and Dr. Hunter will have two main components over the 11-12 month term of his sabbatical (i.e., starting in late July, 2000). During the early part of his visit (i.e., until about December 1st, 2000), our collaboration will center on diffraction education teaching materials. Indeed, I am the editor on a diffraction methods text that Dr. Hunter will be writing for the Royal Society during this time and we hope to have this text substantially completed by Christmas. During the remaining 7-8 months of his sabbatical, our collaboration will be research based. My research is focussed on the synthesis and characterization of novel main group organometallic and coordination complexes, especially those having heterocyclic rings and cages. Indeed, I have over 200 publications in this area and my research on these topics is supported to the extent of approximately $250,000 a year by the UK EPSRC granting agency. This research has been extensively supported by X-ray diffraction using serial, CCD, and Synchrotron diffractometers. We have grown increasingly interested in carrying out high resolution (i.e., charge density) and molecular modeling studies of these

materials to complement our synthetic, spectroscopic, theoretical, and low-resolution diffraction studies. It is in this area that Dr. Hunter, Dr. Slawin (also at St. Andrew's), and myself are planning on establishing our collaboration. Dr. Hunter will carry out high resolution data collections on representative main group ring/cage complexes of ours and will then try to rationalize their know properties in terms of molecular modeling and charge density studies. I expect that this preliminary project will for the basis for a long term collaborative relationship between our crystallography group here at St. Andrew's and Dr. Hunters group at Youngstown State University.

To support our collaboration during the 2000-2001 year, both myself and St. Andrew's and Dr. Hunter and Youngstown State University have already committed significant resources. Youngstown State University has granted Dr. Hunter a sabbatical for the 2000-2001 academic year and will provide support for his preliminary work at YSU before he leaves YSU. I have committed £6,000 from my current EPSRC grants to provide partial support for Dr. Hunter's incremental costs (lodging, utilities, food, travel, etc) during his first four months here at St. Andrew's (i.e., August to November of 2000). We have also committed office and lab space, a substantial block of time on our diffractometers and computers, and "tickets" on the Daresbury synchrotron source for the duration of his stay. However, because of prior commitments to my current students and staff, I am not able to cover his incremental costs for the remainder of his stay here at St. Andrew's. The provision of the requested NSF International Division Collaborative grant funds will allow us to establish the basis for a long term trans-Atlantic partnership!

If you have any questions, please do not hesitate to contact me.

Yours Sincerely,

Prof. J Derek Woollins FRSC C.Chem